Color Molecular-Dynamics for High Density Matter

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We propose a microscopic simulation for quark many-body system based on molecular dynamics. Using color confinement and one-gluon exchange potentials together with the meson exchange potentials between quarks, we construct nucleons and nuclear/quark matter. Statistical feature and the dynamical change between confinement and deconfinement phases are studied with this molecular dynamics simulation.

At high baryon density, the nuclear matter is believed to undergo a phase transition to the quark matter because of the color Debye screening and the asymptotic freedom in quantum chromodynamics (QCD) [1]. In qualitative estimates using the Bag model [2] as well as the strong coupling lattice QCD [3] predict a first order transition at baryon density (ρ) several times over the nuclear matter density ($\rho_0 = 0.17\text{fm}^{-3}$). However, realistic studies of the high density matter based on the first principle lattice QCD simulation are not available yet due to technical difficulties [4]. In this situation, any alternative attempts are welcome to unravel the nature of high density matter. In particular, how the nuclear matter composed of nucleons (which are by themselves composite three-quark objects) dissolve into quark matter is an interesting question to be studied. From the experimental and observational point of view, such transition may occur in high-energy heavy ion collisions [5] and in the central core of neutron stars [6].

In this Letter, we propose a molecular dynamics (MD) simulation [7,8] of a system composed of many constituent quarks [9]. As a first attempt, we carry out MD simulation for quarks with SU(3) color degrees of freedom. Spin and flavor are fixed for simplicity, although there is no fundamental problem to include them. Time evolution of the spatial and color coordinates of quarks are governed by the color confining potential, the perturbative gluon-exchange potential and the meson-exchange potential. The confining potential favors the color neutral cluster (nucleon) at low density. However, as the baryon density increases, the system undergoes a transition to the deconfined quark matter, since the nucleons start to overlap with each other. Our color MD simulation (CMD) is a natural framework to treat such a percolation transition. The meson-exchange potential between quarks, which represent the non-perturbative QCD effects, helps to prevent the system to collapse. Although techniques are quite different, physical idea behind CMD with the meson-exchange potential is quite similar in spirit with the quark-meson coupling (QMC) model extensively used to study the nuclear matter from quarks [10].

We start with a total wave function of the system Ψ as a direct product of single-particle quark wave-functions. The antisymmetrization is neglected at present.

$$\Psi = \prod_{i=1}^{3A} \phi_i(\mathbf{r})\chi_i, \tag{1}$$

$$\phi_i(\mathbf{r}) \equiv (\pi L^2)^{-3/4} \exp[-(\mathbf{r} - \mathbf{R}_i)^2/2L^2 - i\mathbf{P}_i\mathbf{r}], \tag{2}$$

$$\chi_i \equiv \begin{pmatrix} \cos\alpha_i\ e^{-i\beta_i}\ \cos\theta_i \\ \sin\alpha_i\ e^{+i\beta_i}\ \cos\theta_i \\ \sin\theta_i\ e^{i\varphi_i} \end{pmatrix}. \tag{3}$$

Here A is the total baryon number of the system, ϕ_i is a Gaussian wave packet centered around $\mathbf{R}_i$ with momentum $\mathbf{P}_i$ and a fixed width L. χ_i is a coherent state in the color SU(3) space parametrized by four angles, $\alpha_i, \beta_i, \theta_i$ and φ_i. Although general SU(3) vector has six real parameters, the normalization condition $|\chi_i| = 1$ and the unphysical global phase reduce the number of genuine parameters to four. Note that SU(2) spin coherent state parametrized by two angles has been used in the MD simulation of the many-nucleon system with spin [11].

Time evolution of the system is given by solving the equations of motion for $\{\mathbf{R}_i, \mathbf{P}_i, \alpha_i, \beta_i, \theta_i, \varphi_i\}$ obtained from the time-dependent variational principle

$$\frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}, \tag{4}$$

together with the classical Lagrangian,

$$\mathcal{L} = \langle \Psi | i\hbar\frac{d}{dt} - \hat{H} | \Psi \rangle \tag{5}$$

$$= \sum_i [-\dot{\mathbf{P}}_i \mathbf{R}_i + \hbar\dot{\beta}_i \cos 2\alpha_i\ \cos^2\theta_i - \hbar\dot{\varphi}_i \sin^2\theta_i] - H, \tag{6}$$

where $H = \langle \Psi \mid \hat{H} \mid \Psi \rangle$. The explicit form of the equations of motion reads :

$$\dot{\mathbf{R}}_i = \frac{\partial H}{\partial \mathbf{P}_i}, \qquad \dot{\mathbf{P}}_i = -\frac{\partial H}{\partial \mathbf{R}_i}, \tag{7}$$

$$\dot{\beta}_i = -\frac{1}{2\hbar\sin 2\alpha_i\ \cos^2\theta_i}\frac{\partial H}{\partial \alpha_i}, \tag{8}$$

$$\dot{\theta}_i = \frac{1}{2\hbar\sin\theta_i\ \cos\theta_i}\frac{\partial H}{\partial \varphi_i}, \tag{9}$$

$$\dot{\alpha}_i = \frac{1}{2\hbar \sin 2\alpha_i \, \cos^2 \theta_i} \frac{\partial H}{\partial \beta_i} - \frac{\cos 2\alpha_i}{2\hbar \sin 2\alpha_i \, \cos^2 \theta_i} \frac{\partial H}{\partial \varphi_i}, \quad (10)$$

$$\dot{\varphi}_i = -\frac{1}{2\hbar \sin \theta_i \, \cos \theta_i} \frac{\partial H}{\partial \theta_i} + \frac{\cos 2\alpha_i}{2\hbar \sin 2\alpha_i \, \cos^2 \theta_i} \frac{\partial H}{\partial \alpha_i}. \quad (11)$$

As for the color-dependent quark-quark interaction, we employ the one-gluon exchange and the linear confining potentials. To take into account the essential part of the nuclear force, namely, the state independent short range repulsion and the medium range attraction, we include the $\sigma + \omega$ meson-exchange potential acting between quarks following ref. [10]. The total Hamiltonian is written as

$$\hat{H} = \sum_i \sqrt{m^2 + \hat{\mathbf{p}}_i{}^2} + \frac{1}{2} \sum_{i,j\neq i} \hat{V}_{ij}, \quad (12)$$

$$\hat{V}_{ij} = -\sum_{a=1}^{8} t_i^a t_j^a V_{\mathrm{C}}(\hat{r}_{ij}) + V_{\mathrm{M}}(\hat{r}_{ij}), \quad (13)$$

$$V_{\mathrm{C}}(r) \equiv Kr - \frac{\alpha_{\mathrm{s}}}{r}, \quad (14)$$

$$V_{\mathrm{M}}(r) \equiv -\frac{g_{\sigma q}^2}{4\pi} \frac{e^{-\mu_\sigma r}}{r} + \frac{g_{\omega q}^2}{4\pi} \frac{e^{-\mu_\omega r}}{r}, \quad (15)$$

where $t^a = \lambda^a/2$ with λ^a being the Gell-Mann matrices, V_{C} is the confinement and one-gluon exchange terms, and V_{M} is the meson exchange term [12]. We introduce a smooth infrared cutoff to the confining potential in $V_{\mathrm{C}}(r)$ to prevent the long-range interaction beyond the size of the box in which we carry out MD simulations. We choose the cutoff scale $r_{\mathrm{cut}} = 3.0$ fm, which is approximately half of the length of the box. Typical values of the parameters in the quark model for baryons read [12], $m = 350$ MeV (the constituent-quark mass), $\alpha_{\mathrm{s}} = 1.25$ (the QCD fine structure constant), $K = 0.75$ GeV/fm (the string tension). The meson-quark coupling constants $g_{\sigma(\omega)q}$ are estimated from the meson-nucleon couplings $g_{\sigma(\omega)N}$ using the additive quark picture: $g_{\sigma q} = g_{\sigma N}/3 = 3.53$ and $g_{\omega q} = g_{\omega N}/3 = 5.85$. The meson masses are taken to be $\mu_\omega = 782$ MeV and $\mu_\sigma = 550$ MeV.

Some comments are in order here on the evaluation of the matrix elements $H = \langle \Psi \mid \hat{H} \mid \Psi \rangle$.
(i) We have not taken into account the antisymmetrization of quarks in the total wave function. Because of this, the interaction between quarks in a color-singlet baryon is underestimated by factor 4 when one takes the matrix element of $t_i^a t_j^a$. To correct this, we use effective couplings $K^{\mathrm{eff}} = 4K$ and $\alpha_s^{\mathrm{eff}} = 4\alpha_s$ throughout our CMD simulation.
(ii) L (the size of the quark wave-packet) is chosen to be 0.35 fm (corresponding to the r.m.s. radius of the constituent quark of 0.43 fm). This is consistent with the typical value expected from the dynamical breaking of chiral symmetry [13]. This value is to be used for taking the matrix element of the gluonic interaction V_{C}.

On the other hand, the meson-quark coupling is intrinsically non-local, since σ and ω have their own quark structure. Besides, the meson-exchange interaction between nucleons with the nucleon form-factor should be properly reproduced by the superposition of the meson-exchange interaction between quarks. To take into account these facts, we use $L^{\mathrm{eff}} = 0.7$ fm (corresponding to the r.m.s. radius of 0.86 fm) in taking the matrix element of V_{M}.
(iii) $H = \langle \Psi \mid \hat{H} \mid \Psi \rangle$ generally contains a kinetic energy originating from momentum variances of wave packets. However, when the width of the wave packet is fixed as a time-independent parameter, this kinetic energy is spurious and neglected in the present calculation.

Let us now describe how to simulate the simplest three-quark system, namely the nucleon, in CMD. We first search for a three-quark state obeying the color neutrality condition

$$\sum_{i=1}^{3} \langle \chi_i | \lambda^a | \chi_i \rangle = 0 \qquad (a = 1, \cdots, 8). \quad (16)$$

This is satisfied by solving a cooling equation of motion in the color space with a potential proportional to $\sum_{i,j\neq i} \sum_{a=1}^{8} \langle \chi_i | \lambda^a | \chi_i \rangle \langle \chi_j | \lambda^a | \chi_j \rangle$ with random initial values of χ_i. During this cooling procedure, the spatial coordinates of quarks are fixed, e.g. at the three corners of a triangle.

If we start with three quarks in triangular position obtained above and kick each quark by a same amount of energy keeping the total momentum zero, the quarks start to have a breathing motion in 2-dimensional plane. Since the total color is conserved, the color-neutrality is maintained during this time evolution.

By an initial kick to give the time-averaged kinetic energy of 74 MeV, the total energy of the nucleon become 1269 MeV. Accordingly, the r.m.s. radius of the nucleon reads 0.46 fm in terms of L (which corresponds to the size of the quark-core of the nucleon) or 0.87 fm in terms of L^{eff} (which corresponds to the physical nucleon size for meson-exchange interaction). The "nucleon" here is certainly a semiclassical object which should be regarded as a mixture of the ground and excited states of three quarks. We use a collection of these nucleons as an initial condition for the CMD simulation of many quarks. Since the interaction among quarks in matter will eventually randomize the internal motion of quarks in the initial nucleon, the way how we kick the quarks does not matter for the final result.

Now, let us study the phase change from the confined hadronic system to the deconfined quark matter. We simulate the infinite matter under the periodic boundary condition and see how the system responds to the change of the baryon density as well as to the energy deposition from outside.

To start with, nucleons constructed as above are randomly distributed in a box with the periodic boundary condition. At this stage, the total system is in its excited state. The minimum energy state of matter is obtained by the frictional cooling procedure, namely we solve a cooling equation of motion with frictional terms. During the cooling, spatial and color motion of quarks in the nucleon are artificially frozen, and the following equations are solved:

$$\dot{\mathbf{R}}_i = \frac{1}{3} \sum_{j \in \{i\}} \left[\frac{\partial H}{\partial \mathbf{P}_j} + \mu_R \frac{\partial H}{\partial \mathbf{R}_j} \right], \tag{17}$$

$$\dot{\mathbf{P}}_i = \frac{1}{3} \sum_{j \in \{i\}} \left[-\frac{\partial H}{\partial \mathbf{R}_j} + \mu_P \frac{\partial H}{\partial \mathbf{P}_j} \right], \tag{18}$$

$$\dot{\alpha}_i = \dot{\beta}_i = \dot{\theta}_i = \dot{\varphi}_i = 0, \tag{19}$$

where μ_R and μ_P are damping coefficients with negative values and $\{i\}$ means a set of three quarks in a nucleon to which i belongs. Under this cooling procedure, the system approaches to a stable configuration with minimum energy. The system does not collapse due to the repulsive part of the meson exchange potential V_M.

After the system reached its energy-minimum by the cooling, internal color and spatial motion of quarks are turned on and the normal equation of motion is solved for several tens of fm/c so that the system gets equilibrated. To study the excited state of the system, extra random motion is also given to the nucleons so that the system has a certain excitation energy.

We judge the confinement/deconfinement by the following criterion. If three quarks are within a certain distance d_{cluster} and are white with an accuracy ε, these quarks are said to be confined. This can be formulated as

$$\begin{cases} |\mathbf{R}_i - \mathbf{R}_j| < d_{\text{cluster}} \quad (i,j=1,2,3), \\ \sum_{a=1}^{8} \left[\sum_{i=1}^{3} \langle \chi_i | \lambda^a | \chi_i \rangle \right]^2 < \varepsilon. \end{cases} \tag{20}$$

All quarks are checked by this criterion without duplications. The actual numbers we use are $d_{\text{cluster}} = 1$ fm and $\varepsilon = 0.05$.

Snapshots of matter in equilibrium for different excitation energies per quarks (E^*) are displayed in Fig. 1. Quarks in the confined states are shown with thin colors and those in the deconfined state with thick colors. As E^* increases, number of deconfined quarks increases as expected. However, some deconfined quarks still form three-quark clusters even for large E^*. This implies that the deconfinement is caused not only by disintegration or percolation of clusters in the coordinate space but also by the color excitation inside each cluster.
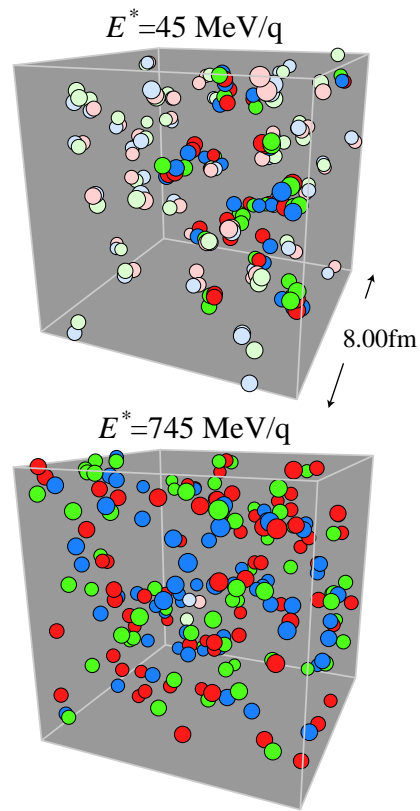

FIG. 1. Perspective of matter with different excitation energies per quark E^* at baryon density $0.78\rho_0$. Particles with thin (thick) colors indicate quarks in the confined (deconfined) state.

Figure 2 shows a "confined ratio of quarks", $R \equiv$ (number of confined quarks)/(total quark number). At $E^* = 0$, hadronic matter and the quark matter are well characterized by R although no sudden transition of R between the two phases is observed. For $E^* > 200$ MeV/q, R is less than 20% for all densities.

To study the "thermal" property of the system, we fit the kinetic energy distribution of quarks by the classical Boltzmann distribution. Then, we can define an effective temperature T^* for given E^*. Note that T^* is not really a physical temperature of the system, but is a measure of the averaged kinetic energy per quark. In Fig. 3, plotted is T^* as a function of E^*. For $E^* > 300$ MeV/q, T^* depends almost linearly on E^* irrespective of baryon density. However, for $E^* = 100 \sim 200$ MeV/q, T^* for low-density matter increases rather slowly as a function of E^*. In fact, this corresponds exactly to the region where the confined ratio of low-density matter changes in Fig. 2. This implies that, during the deconfinement process, the energy deposit from outside is consumed to melt the confined clusters (nucleons), which suppresses the effective temperature T^*.
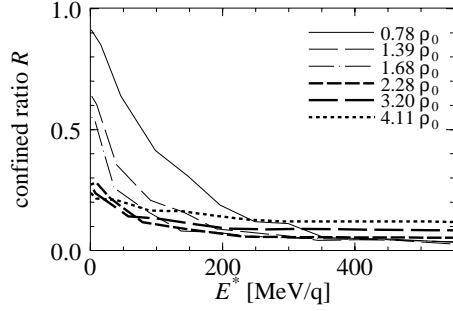
FIG. 2. Confined ratio of quarks as a function of E^* for several different baryon densities.
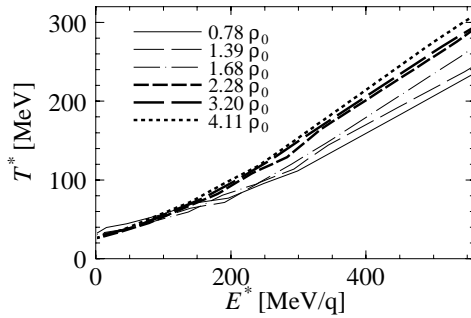

FIG. 3. Baryon density and excitation energy dependence of the effective temperature extracted from the Boltzmann fit of the kinetic energy distribution.

In summary, we have proposed a color molecular dynamics (CMD) simulation of the system with many constituent quarks. The system is approximated by the product of the wave packets with SU(3) color coherent state. Adopting the effective interaction between quarks, we study the transition from the nuclear matter to quark matter under the periodic boundary condition. At low baryon density (ρ) and low excitation energy (E^*), the system is in the confined phase where most of the quarks are hidden inside the color singlet nucleons. However, as we increase ρ and/or E^*, the partial deconfinement takes place due to the disintegration of color-singlet clusters both in the coordinate space and in the color space. This can be seen explicitly by the confined ratio and effective temperature in Fig.2 and Fig.3.

The results of this paper are still in the qualitative level. The refinement of interaction parameters, and the inclusion of flavor and spin degrees of freedom as well as anti-quarks are necessary for more quantitative discussions. The use of the antisymmetrized quark wave function is also an important future problem [14]. The medium modification of the constituent-quark mass should be also considered in relation to the partial restoration of chiral symmetry. In spite of all

these reservations, the method proposed in this paper gives a starting point to study the statistical feature of the hadron-quark transition as well as to examine finite nuclei and the dynamics of heavy-ion collisions. Some preliminary simulation on the latter problem has been reported in [9].

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